Carbonaceous Chemistry for Computational Modeling (C3M)

Description

C3M is chemistry management software focused on computational modeling of reacting systems. The primary function of C3M is to provide direct links between reliable sources of kinetic information (kinetic modeling software, databases, and literature) and commonly used CFD software such as MFIX, FLUENT, and BARRACUDA with minimal effort from the user. C3M also acts as a virtual kinetic laboratory to allow a CFD practitioner or researcher to evaluate complex, large sets of kinetic expressions for reliability and suitability and can interact with spreadsheet and process models. Once the chemical model is built within C3M, the software also allows the user to directly export the model to CFD software and/or a detailed report of all equations and values used to build the chemical model.

Benefits

The primary benefit of using C3M is speed and accuracy in building kinetic models for computational modeling. Traditionally, the process of building kinetic models for computational applications was extremely time consuming and expensive. Practitioners would have to search literature, code the kinetics into the computational model, debug the code, build test cases, and validate the cases against experimental information before getting to the process of modeling the desired system. C3M eliminates this time consuming and expensive process by linking to sources of kinetic information which are known to be reliable and then automatically building the input for computational models.

CONTACTS

Jenny Tennant
Office of Coal and Power R&D
National Energy Technology Laboratory
3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26505-0880
304-285-4830
jenny.tennant@netl.doe.gov

Madhava Syamlal
Office of Research and Development
National Energy Technology Laboratory
3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26505-0880
304-285-4685
madhava.syamlal@netl.doe.gov

Dirk Van Essendelft
Computational Science Division
National Energy Technology Laboratory
3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-5231
dirk.vanessendelft@netl.doe.gov

NETL-RUA COLLABORATORS

University Research Corporation
West Virginia University

NATIONAL ENERGY TECHNOLOGY LABORATORY

Albany, OR • Anchorage, AK • Morgantown, WV • Pittsburgh, PA • Sugar Land, TX

Website: www.netl.doe.gov

Customer Service: 1-800-553-7681

U.S. DEPARTMENT OF
ENERGY

Successes

NETL has done several successful CFD models for third party, industrial partners through cooperative research and development agreements (CRADA's). Since the inception of C3M, it has played a pivotal role in shortening the turnaround time to obtaining CFD results. Recently, NETL completed detailed CFD modeling of a new, industrial scale TRIG reactor for gasification. C3M was used to construct the chemistry models within the CFD simulations and reduced the turnaround time from several months to several weeks and eliminated the need for detailed chemistry validation. C3M saved thousands of man hours of development and several hundred computational hours which significantly reduced the cost for the client. NETL is continuing to work with industry in the area of modeling reacting systems to accelerate commercial-scale development and reduce uncertainties associated with commercial deployment.
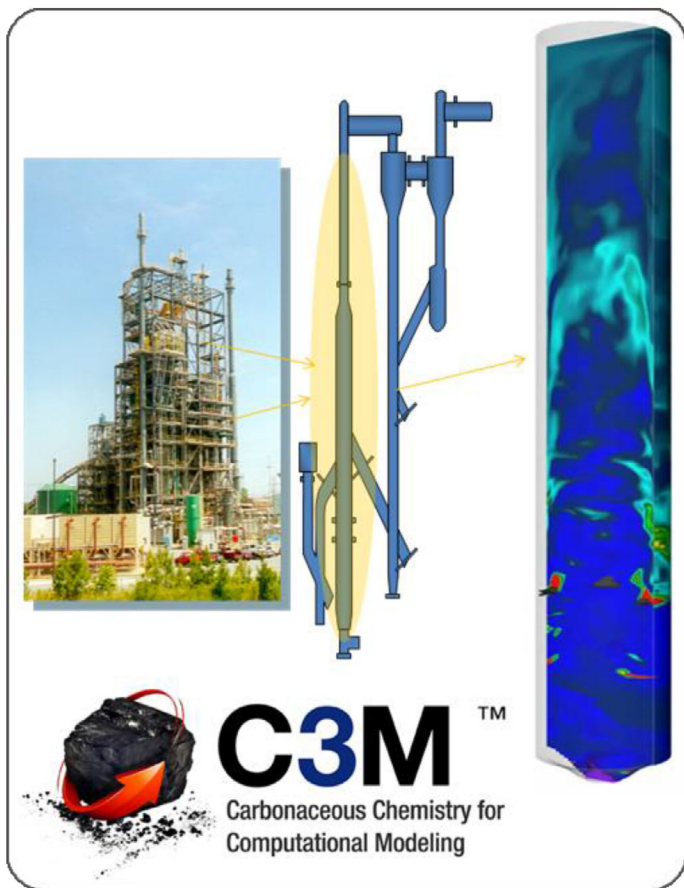
Existing Capabilities

- Direct links to kinetic data sources termed "Kinetic Packages"
  - NETL's METC Gasifier Advanced Simulation (MGAS)
  - Niksa Energy Associate's PC Coal Lab® (PCCL)
  - University of Utah's Chemical Percolation Devolatilization (CPD)
  - Advanced Fuel Research's Functional-Group, Depolymerization, Vaporization, Cross-linking (FG-DVC)
  - NETL Co-Pyrolysis Data
- Chemical expressions and kinetic rates for gasification
  - Moisture Release, Pyrolysis (Primary, Secondary, Tar Cracking), Char Gasification, Soot Gasification, Water Gas-Shift, Gas Phase Combustion, Char Oxidation, Soot Oxidation, Tar Oxidation
- Thermodynamic data for "Pseudo Species"
- Graphical plots showing product composition and rates for comparison among different kinetic models
- A comprehensive report detailing all equations in the chemical system
- Formatted input files for ANSYS FLUENT, CPFD BARRACUDA, and NETL's MFIX
- Easy, intuitive, and reliable graphical user interface
- Kinetic data for fuel flexible systems
  - Co-pyrolysis experimental data for PRB and Southern Pine is included

Capabilities under Development

- Advanced visualization capabilities
  - "Click and Run" drop tube gasifier and TGA through NETL's MFIX
  - Will allow visualization of complete chemistry model with heat and mass transfer included
  - Will allow users to directly compare CFD results to most common types of experiments within C3M
- Uncertainty Quantification
  - Will produce response surfaces and PDF functions for CFD codes
- Include expanded kinetic datasets
  - Sulfur removal, mercury capture, chemical looping and oxy-combustion, etc
  - Co-gasification data for PRB and Southern Pine
- Increased breadth of validation test cases
  - Used to continually refine kinetic models and improve predictive accuracy